

# A transport equation for the scalar dissipation in reacting flows with variable density: first results

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## 1. Motivation and objectives

### 1.1 Introduction

Although the different regimes of premixed combustion are not well defined, most of the recent developments in turbulent combustion modeling are led in the so-called flamelet regime. The goal of these models is to give a realistic expression to the mean reaction rate  $\langle \dot{w} \rangle$ . Several methods can be used to estimate  $\langle \dot{w} \rangle$ . Bray and coworkers (Libby & Bray 1980, Bray 1985, Bray & Libby 1986) express the instantaneous reaction rate by means of a flamelet library and a frequency which describes the local interaction between the laminar flamelets and the turbulent flow field. In another way, the mean reaction rate can be directly connected to the flame surface density  $\langle \Sigma \rangle$ . This quantity can be given by the transport equation of the coherent flame model initially proposed by Marble & Broadwell 1977 and developed elsewhere (Pope 1988, Candel & Poinso 1990, Trouvé & Poinso 1992, Bidaux *et al.* 1993). The mean reaction rate,  $\langle \dot{w} \rangle$ , can also be estimated thanks to the evolution of an arbitrary scalar field  $G(\mathbf{x}, t) = G_0$  which represents the flame sheet.  $G(\mathbf{x}, t)$  is obtained from the  $G$ -equation proposed by Williams 1985, Kerstein *et al.* 1988 and Peters 1993. Another possibility proposed in a recent study by Mantel & Borghi 1991, where a transport equation for the mean dissipation rate  $\langle \epsilon_c \rangle$  of the progress variable  $c$  is used to determine  $\langle \dot{w} \rangle$ .

In their model, Mantel & Borghi 1991 considered a medium with constant density and constant diffusivity in the determination of the transport equation for  $\langle \epsilon_c \rangle$ . A comparison of different flamelet models made by Duclos *et al.* 1993 shows the realistic behavior of this model even in the case of constant density. Our objective in this present report is to present preliminary results on the study of this equation in the case of variable density and variable diffusivity. Assumptions of constant pressure and a Lewis number equal to unity allow us to significantly simplify the equation. A systematic order of magnitude analysis based on adequate scale relations is performed on each term of the equation. As in the case of constant density and constant diffusivity, the effects of stretching of the scalar field by the turbulent strain field, of local curvature, and of chemical reactions are predominant. In this preliminary work, we suggest closure models for certain terms, which will be validated after comparisons with DNS data.

### 1.2 The role of scalar dissipation for premixed turbulent combustion

For the prediction of chemical reactions in premixed media, the dissipation time scale of the concentration (or the temperature) fluctuations  $\tau_c$  and of the turbulent kinetic energy  $\tau_t$  are crucial quantities. Nevertheless, in most turbulent combustion

models (flamelets models, presumed pdf approach) where these scales are taken into account, proportionality between these quantities is very often assumed. Although, numerous experimental studies show that the ratio of these two scales is not a constant and varies for different flows (see Beguier *et al.* 1978).

One way of calculating the dissipation time scale of a scalar is to use a transport equation for the dissipation of the fluctuations of this scalar  $\langle \epsilon_c \rangle = \langle d \frac{\partial c'}{\partial x_i} \frac{\partial c'}{\partial x_i} \rangle$  (where  $d$  is the molecular diffusivity and  $c'$  the fluctuation of  $c$ ;  $c$  is defined to be equal to 1 in the burnt gases and to 0 in the fresh gases). Starting from the studies of Zeman & Lumley 1976, Borghi & Dutoya 1978 used this equation to investigate the case of a steady premixed flame. But the use of such an equation requires the modeling of many terms and very little knowledge exists to assess the adequacy of these models.

More recently, Mantel & Borghi 1991 have developed a transport equation for  $\langle \epsilon_c \rangle$  in the case of constant density and constant diffusivity. An order of magnitude analysis based on appropriate scale relations shows that the effects of stretching of the concentration field by the small scales of turbulence and the effects of local curvature are predominant. The authors present new closures for these terms in order to take into account the presence of laminar flamelet within the flow.

The applications of such an equation are significant and of fundamental interest:

- 1- In the particular case of high Damköhler number,  $Da = \tau_t / \tau_{ch}$  where  $\tau_{ch}$  is a chemical time scale, Bray & Moss 1977 and Borghi 1978 have demonstrated that  $\langle \dot{w} \rangle$  and  $\langle \epsilon_c \rangle$  are directly related:

$$\langle \dot{w} \rangle = \frac{\langle \epsilon_c \rangle}{\frac{1}{2} - b_0} \quad (1.1)$$

where,

$$b_0 = \frac{\int_0^1 c \dot{w}(c) dc}{\int_0^1 \dot{w}(c) dc}.$$

In accordance with Bray & Moss 1977, the equation for  $\langle \epsilon_c \rangle$  leads to a transport equation for the mean reaction rate and to a new formulation of the well known Eddy Break-Up model.

- 2- Moreover, in the flamelet regime,  $\langle \epsilon_c \rangle$  and  $\langle \Sigma \rangle$  can be directly connected by  $\langle \epsilon_c \rangle \propto S_L \langle \Sigma \rangle$  (see Borghi 1990), where  $S_L$  is the laminar flame velocity. Thus, a transport equation for  $\langle \Sigma \rangle$  is obtained in a different way from those proposed by other studies (Marble & Broadwell 1977, Candel & Poinso 1990, Trouvé & Poinso 1992, Bidaux *et al.* 1993).
- 3- Furthermore, the knowledge of the dissipation time scale for the scalar allows Mantel *et al.* 1993 to propose a new model for the equation for the correlation  $\langle u_i' c' \rangle$  which is another crucial problem in turbulent modeling that is often underestimated.

## 2. Accomplishments

We present in this section the different steps and assumptions leading to the equation for  $\langle \epsilon_c \rangle$ .

The methodology chosen here to calculate the transport equation for  $\langle E_c \rangle$  is to first establish the instantaneous equation for  $E_c = d \frac{\partial c}{\partial x_i} \frac{\partial c}{\partial x_i}$ . An averaging operation and an order of magnitude analysis of this equation will lead directly to the equation for  $\langle \epsilon_c \rangle$ .

### 2.1 Preliminaries

In order to determine the transport equation for  $E_c$ , some assumptions are made. A perfectly premixed medium is considered and a single chemical reaction occurs in the flow which can be described by:  $F_{\text{uel}} + O_{\text{xydizer}} \rightarrow P_{\text{roducts}}$ .

From the instantaneous transport equation for the progress variable  $c$ :

$$\frac{\partial c}{\partial t} + U_k \frac{\partial c}{\partial x_k} = \frac{1}{\rho} \frac{\partial}{\partial x_k} \left( \rho d \frac{\partial c}{\partial x_k} \right) + \dot{w} \quad (2.1)$$

The transport equation for  $E_c$  is obtained by differentiating Eq. (2.1) with respect to  $x_i$  and by multiplying the result by  $dc_{,i}$ , where  $c_{,i}$  represents  $\frac{\partial c}{\partial x_i}$ . After some algebra, the transport equation for  $E_c$  leads to:

$$\begin{aligned} \frac{\partial E_c}{\partial t} + U_k \frac{\partial E_c}{\partial x_k} &= c_{,i} c_{,i} d_{,i} + U_k d_{,k} c_{,i} c_{,i} - 2dc_{,i} c_{,k} \frac{\partial U_k}{\partial x_i} + \frac{1}{\rho} \frac{\partial}{\partial x_k} \left( \rho d \frac{\partial E_c}{\partial x_k} \right) \\ &+ 2dc_{,i} c_{,k} \frac{\partial}{\partial x_i} \left( \frac{1}{\rho} (\rho d)_{,k} \right) - E_c \frac{\partial^2 d}{\partial x_k^2} - 2dd_{,k} \frac{\partial c_{,i} c_{,i}}{\partial x_k} - \frac{d}{\rho} \rho_{,k} d_{,k} c_{,i} c_{,i} \\ &- d_{,k} d_{,k} c_{,i} c_{,i} + 2dd_{,i} c_{,i} \frac{\partial^2 c}{\partial x_k^2} - 2d^2 \frac{\partial c_{,i}}{\partial x_k} \frac{\partial c_{,i}}{\partial x_k} + 2dc_{,i} \dot{w}_{,i} \end{aligned} \quad (2.2)$$

Obviously, Eq. (2.2) involves unclear correlations and cannot be used directly. New assumptions are needed in order to simplify Eq. (2.2) and to clarify the physical meaning of its terms. Let us consider setting the Lewis number equal to unity, no heat losses, and a constant pressure. Concerning this last assumption, even if a pressure drop occurs across a laminar flame, it is so weak that the density variations are essentially due to temperature variation across the flame front. This assumption could only be put into question in case of strong pressure waves spreading into the flame front (i.e. knock in I.C. engines).

In case of a Lewis number equal to unity and no heat losses, the temperature and the progress variable are directly related by:

$$T = T_0(1 + \theta c) \quad (2.3)$$

where  $\theta$  is the heat release parameter:  $\theta = \frac{T_{ad} - T_0}{T_0}$ ,  $T_{ad}$  and  $T_0$  represent respectively the adiabatic temperature and the temperature of the fresh gases.

Due to assumptions of constant pressure, unit Lewis number, and no heat losses, density and diffusivity derivatives can be related to the progress variable derivatives which allow to simplify Eq. (2.2).

The assumption of constant pressure and Eq. (2.3) imply:

$$\rho_{,k} = -\rho \frac{\theta}{1 + \theta c} c_{,k} \quad (2.4)$$

$$\frac{\partial \rho_{,i}}{\partial x_k} = 2\rho \frac{\theta^2}{(1 + \theta c)^2} c_{,i} c_{,k} - \rho \frac{\theta}{1 + \theta c} \frac{\partial c_{,i}}{\partial x_k} \quad (2.5)$$

and allow us to replace in Eq. (2.2) the density derivatives by the progress variable derivatives.

The diffusivity derivatives can be solved by considering that the dynamic viscosity  $\mu$  is only a function of the temperature, for example:

$$\mu = \mu_0 \left( \frac{T}{T_0} \right)^b \quad (2.6)$$

where  $b$  is a constant equal to 0.76. The dynamic viscosity at temperature  $T_0$  is denoted by  $\mu_0$ . Thus, the first and second derivatives for the molecular diffusivity can also be related to the first and second derivatives of the progress variable:

$$d_{,k} = (1 + b)d \frac{\theta}{1 + \theta c} c_{,k} \quad (2.7)$$

$$\frac{\partial^2 d}{\partial x_k^2} = b(b + 1) \frac{\theta^2}{(1 + \theta c)^2} dc_{,k} c_{,k} + (b + 1) \frac{\theta}{1 + \theta c} \frac{\partial^2 c}{\partial x_k^2} \quad (2.8)$$

$$\frac{\partial d_{,i}}{\partial x_k} = b(b + 1) \frac{\theta^2}{(1 + \theta c)^2} dc_{,i} c_{,k} + (b + 1) \frac{\theta}{1 + \theta c} \frac{\partial c_{,i}}{\partial x_k} \quad (2.9)$$

Substituting these new expressions for the derivatives of the density and molecular diffusivity, Eq. (2.2) becomes:

$$\begin{aligned} \rho \frac{\partial E_c}{\partial t} + \rho U_k \frac{\partial E_c}{\partial x_k} &= \frac{\partial}{\partial x_k} \left( \rho d \frac{\partial E_c}{\partial x_k} \right) - 2\rho dc_{,i} c_{,k} \frac{\partial U_k}{\partial x_i} + (1 + b)\rho E_c \frac{\partial U_k}{\partial x_k} \\ &\quad - 2b\rho \frac{\theta^2}{(1 + \theta c)^2} E_c^2 + (1 + b)\rho \frac{\theta}{1 + \theta c} d E_c \frac{\partial^2 c}{\partial x_k^2} \\ &\quad - 2(2 + b)\rho \frac{\theta}{1 + \theta c} d^2 c_{,i} c_{,k} \frac{\partial c_{,i}}{\partial x_k} - 2\rho d^2 \frac{\partial c_{,i}}{\partial x_k} \frac{\partial c_{,i}}{\partial x_k} + 2\rho dc_{,i} \dot{w}_{,i} \end{aligned} \quad (2.10)$$

In Eq. (2.10), derivatives of density and diffusivity disappear and a physical meaning of the terms of Eq. (2.10) can be seen more clearly. But before we give physical meanings to these terms and propose closures, averaging operations and an order of magnitude analysis are performed. We will see that the instantaneous gradients of  $c$  are predominant and allow us to derive an equation for  $\langle \epsilon_c \rangle$ .

## 2.2 Averaging and order of magnitude analysis

## 2.2.1 Preliminaries and scale relations

First, we decompose the velocity and the progress variable into a mean value and a fluctuating component (i.e. for  $c$ , we have  $c = \langle c \rangle + c'$  where  $\langle c \rangle = \frac{\rho c}{\bar{\rho}}$  is the Favre averaging, and by definition  $\langle c' \rangle = 0$ ). The order of magnitude analysis needs appropriate scale relations which take into account the presence of chemical reactions in the fluid. For the gradient of the velocity, the approach of Tennekes & Lumley 1972 (pp 88-92) for the vorticity equation is retained. These scale relations are  $\frac{\partial \langle U_k \rangle}{\partial x_i} \propto \frac{u'}{l_t}$  and  $\frac{\partial u'_k}{\partial x_i} \propto \frac{u'}{\lambda}$  where  $l_t$  and  $\lambda$  are respectively the integral length scale and the Taylor microscale of the turbulence.

For the quantities related to the concentration flow field, the problem is more subtle. Because chemical reactions occur within the flow, we have to take into account the existence of flamelets in the turbulent flow field in order to estimate the scale relations, and we must also know the pdf (probability density function) of  $c$  for the averaging operation.

In the limit of very large  $Da$ , this pdf is essentially composed of two peaks corresponding to the fresh and burnt gases:

$$P(c) = \delta_0 \delta(c) + \gamma f(c) + \delta_1 \delta(1 - c) \quad (2.11)$$

The constant  $\gamma$  in Eq. (2.11) must to be proportional to  $Da^{-1}$  as demonstrated by Bray & Moss 1977. This can be easily justified by noting that in the case of very fast chemical reactions ( $\tau_c \rightarrow 0$ ), the instantaneous reaction rate tends to infinity ( $\tau_{ch}^{-1} = \int_0^1 \dot{w}(c) dc$ ) while the mean reaction rate, defined by:

$$\langle \dot{w} \rangle = \int_0^1 \dot{w}(c) P(c) dc \quad (2.12)$$

has to remain finite (since  $\dot{w}(0) = 0$ ,  $\dot{w}(1) = 0$ ). This point has a strong impact on the order of magnitude analysis on terms where concentration gradients appear.

We now go back to the gradients of the progress variable. Mantel and Borghi 1991 proposed to relate mean gradients to the integral length scale  $\frac{\partial \langle c \rangle}{\partial x_i} \propto \frac{\langle c'^2 \rangle^{1/2}}{l_t}$  and instantaneous gradients to the laminar flame thickness  $\delta_L$ :  $\frac{\partial c'}{\partial x_i} \propto \frac{\langle c'^2 \rangle^{1/2}}{\delta_L}$ .

The relations  $S_L \propto (d/\tau_{ch})^{1/2}$  and  $\delta_L \propto (d\tau_{ch})^{1/2}$  are also needed in this analysis. As an example, we can examine the case of  $\langle E_c \rangle$  itself. By definition, we have:

$$\langle E_c \rangle = \int_0^1 dc_{,i} c_{,i} P(c) dc \equiv d \frac{\langle c'^2 \rangle}{\delta_L^2} Da^{-1} \equiv \frac{\langle c'^2 \rangle}{\tau_t} Da^0 Re_t^0 \quad (2.13)$$

where,  $Re_t$  is the Reynolds number based on the integral length scale  $Re_t = u' l_t / \nu$ .

Decomposing  $c$  into a mean value and a fluctuating component,  $\langle E_c \rangle$  can be developed in different terms:

$$\langle E_c \rangle = \langle dc_{,i}c_{,i} \rangle = \langle d \rangle \langle c_{,i} \rangle \langle c_{,i} \rangle + 2 \langle dc'_{,i} \rangle \langle c_{,i} \rangle + \langle dc'_{,i}c'_{,i} \rangle \quad (2.14)$$

$$\text{Re}_i^{-1} Da^0 \quad \text{Re}_i^{-1/2} Da^{-1/2} \quad \text{Re}_i^0 Da^0$$

and we can conclude that in the case of large Reynolds and Damköhler numbers, only the last term of Eq. (2.14) has to be retained:

$$\langle E_c \rangle \equiv \langle dc'_{,i}c'_{,i} \rangle = \langle \epsilon_c \rangle \quad (2.15)$$

This explains why we can derive an equation for  $\langle \epsilon_c \rangle$  from the equation for  $\langle E_c \rangle$ .

### 2.2.2 The averaged equation

The separation of the velocity  $U_k$  and the progress variable  $c$  into a mean value and a fluctuation leads to a large number of correlations and new terms in the Eq. (2.10). However, the order of magnitude analysis permits an investigation concerning the relative importance of the terms of the equation and allows removal of these terms which are negligible.

After a systematic study of each term in Eq. (2.10), we obtain:

$$\begin{aligned} \frac{\partial}{\partial t} \bar{\rho} \langle \epsilon_c \rangle + \frac{\partial}{\partial x_k} (\bar{\rho} \langle U_k \rangle \langle \epsilon_c \rangle) &= \frac{\partial}{\partial x_k} \left( \bar{\rho} \langle d \frac{\partial \epsilon_c}{\partial x_k} \rangle \right) - \frac{\partial}{\partial x_k} \left( \bar{\rho} \langle u'_k \epsilon_c \rangle \right) + b \bar{\rho} \langle \epsilon_c \rangle \frac{\partial \langle U_k \rangle}{\partial x_k} \\ \text{(I)} \quad \text{(II)} \quad \text{Re}_i^0 Da^0 &\quad \text{(III)} \quad \text{Re}_i^{-1/2} Da^{1/2} \quad \text{(IV)} \quad \text{Re}_i^0 Da^0 \quad \text{(V)} \quad \text{Re}_i^0 Da^0 \\ &+ b \bar{\rho} \langle \epsilon_c \frac{\partial u'_k}{\partial x_k} \rangle - \bar{\rho} \left( \langle dc_{,i}c_{,k} \rangle \frac{\partial \langle U_k \rangle}{\partial x_i} \right)_{i \neq k} - \bar{\rho} \left( \langle dc_{,i}c_{,k} \frac{\partial u'_k}{\partial x_i} \rangle \right)_{i \neq k} \\ \text{(VI)} \quad \text{Re}_i^{1/2} Da^0 &\quad \text{(VII)} \quad \text{Re}_i^0 Da^0 \quad \text{(VIII)} \quad \text{Re}_i^{1/2} Da^0 \\ &- 2b \bar{\rho} \left\langle \frac{\theta^2}{(1 + \theta c)^2} \epsilon_c^2 \right\rangle - 4b \bar{\rho} \langle c_{,i} \rangle \left\langle \frac{\theta^2}{(1 + \theta c)^2} dc_{,i} \epsilon_c \right\rangle \\ \text{(IX)} \quad \text{Re}_i^0 Da^1 &\quad \text{(X)} \quad \text{Re}_i^{-1/2} Da^{1/2} \\ &- 2(b + 3) \bar{\rho} \langle c_{,i} \rangle \left\langle \frac{\theta}{1 + \theta c} d^2 c'_{,i} \frac{\partial^2 c'}{\partial x_k^2} \right\rangle - (b + 3) \bar{\rho} \left\langle \frac{\theta}{1 + \theta c} d \epsilon_c \frac{\partial^2 c'}{\partial x_k^2} \right\rangle \\ \text{(XI)} \quad \text{Re}_i^{-1/2} Da^{1/2} &\quad \text{(XII)} \quad \text{Re}_i^0 Da^1 \\ &- 2 \bar{\rho} \left\langle d^2 \frac{\partial c_{,i}}{\partial x_k} \frac{\partial c_{,i}}{\partial x_k} \right\rangle + 2 \bar{\rho} \langle c_{,i} \rangle \langle d \dot{w}_{,i} \rangle + 2 \bar{\rho} \langle c'_{,i} d \dot{w}'_{,i} \rangle \\ \text{(XIII)} \quad \text{Re}_i^0 Da^1 &\quad \text{(XIV)} \quad \text{Re}_i^{-1/2} Da^{1/2} \quad \text{(XV)} \quad \text{Re}_i^0 Da^1 \end{aligned} \quad (2.16)$$

Some physical interpretations are proposed for the terms appearing in Eq. (2.16). From left to right, the following terms appear:

- (I) accumulation
- (II) convection

- (III) molecular diffusion
- (IV) turbulent diffusion
- (V) production (or destruction) due to expansion (or compression) of the mean velocity field
- (VI) production (or destruction) due to expansion (or compression) of the turbulent flow field
- (VII) production due to mean velocity gradient
- (VIII) production by stretching of the concentration field by the turbulent strain field
- (IX) destruction
- (X) production (or destruction) due to mean concentration gradients
- (XI) production (or destruction) due to local curvature effects
- (XII) destruction due to local curvature effects
- (XIII) destruction due to molecular dissipation
- (XIV) production (or destruction) due to chemical reactions
- (XV) production (or destruction) due to chemical reactions

### 2.3 First closure attempts

In this section, we present closures for some of the terms of Eq. (2.16). Because this study is in a preliminary phase, closure models do not exist for some terms but are currently under investigation.

- The turbulent diffusion term (IV) is closed by relating the correlation  $\langle u'_k \epsilon_c \rangle$  to a turbulent diffusion coefficient  $d_t$  and to the gradient of  $\langle \epsilon_c \rangle$ :

$$-\langle u'_k \epsilon_c \rangle = \frac{d_t}{\sigma_c} \frac{\partial \langle \epsilon_c \rangle}{\partial x_k} \quad (2.17)$$

where  $\sigma_c$  is a Schmidt number.

- The term due to expansion or compression (VI) can not be closed easily. The sign of this correlation depends on the local velocity field. This sign could be determined by analysis of DNS results.
- The production term due to mean velocity gradient (VII) can be modeled as in Zeman & Lumley 1976:

$$-\bar{\rho} \left( \langle dc_{,i} c_{,k} \rangle \frac{\partial \langle U_k \rangle}{\partial x_i} \right)_{i \neq k} = C_{P_V} \bar{\rho} \langle \epsilon_c \rangle \frac{\langle u'_i u'_k \rangle}{k} \frac{\partial \langle U_k \rangle}{\partial x_i} \quad (2.18)$$

where  $C_{P_V} = 1.0$  and  $k$  represents the turbulent kinetic energy.

- The production by stretching of the concentration field due to the turbulent strain field (VIII) can be modeled as in the case with constant density. Because the sign of this correlation seems to be negative (see the experimental results of Antonia & Browne 1983), this term represents a production of  $\langle \epsilon_c \rangle$ . Thus, the model proposed by Mantel & Borghi 1991 is still valid:

$$-\bar{\rho} \left( \langle dc_{,i} c_{,k} \rangle \frac{\partial u'_k}{\partial x_i} \right)_{i \neq k} = \alpha_0 \bar{\rho} Re_i^{1/2} \frac{\langle \epsilon_c \rangle}{\tau_i} \quad (2.19)$$

where  $\alpha_0$  is a constant ( $\alpha_0 = 0.9$ ).

- The term  $-2b\bar{\rho}\langle\frac{\theta^2}{(1+\theta c)^2}\epsilon_c^2\rangle$  is always negative and represents a destruction of  $\langle\epsilon_c\rangle$ . We propose as a first approximation:

$$2b\bar{\rho}\langle\frac{\theta^2}{(1+\theta c)^2}\epsilon_c^2\rangle = R_1\bar{\rho}\frac{\theta^2}{(1+\theta\langle c\rangle)^2}\langle\epsilon_c\rangle^2 \quad (2.20)$$

where  $R_1$  is a constant. Its value could be estimated from DNS results.

- The production (or destruction) due to mean concentration gradients  $4b\bar{\rho}\langle c,i\rangle\langle\frac{\theta^2}{(1+\theta c)^2}dc_{,i}\epsilon_c\rangle$  can not be easily modeled. More information concerning the correlation  $c_{,i}\epsilon_c$  has to be extracted from DNS or analytical study.
- The term  $-2(b+3)\bar{\rho}\langle c,i\rangle\langle\frac{\theta}{1+\theta c}d^2c'_{,i}\frac{\partial^2c'}{\partial x_k^2}\rangle$  is a production (or a destruction) of  $\langle\epsilon_c\rangle$ . No clear closure can be proposed, and more investigation must be pursued.
- The term  $(b+3)\bar{\rho}\langle\frac{\theta}{1+\theta c}d\epsilon_c\frac{\partial^2c'}{\partial x_k^2}\rangle$  is a production (or destruction) of  $\langle\epsilon_c\rangle$  due to local curvature effects. Following the closure proposed by Mantel & Borghi 1991 for the curvature, we propose:

$$(b+3)\bar{\rho}\langle\frac{\theta}{1+\theta c}d\epsilon_c\frac{\partial^2c'}{\partial x_k^2}\rangle = R_2\bar{\rho}\frac{\theta}{1+\theta\langle c\rangle}\frac{\langle\epsilon_c\rangle^2}{\langle c'^2\rangle^{1/2}}Re_t^{1/4} \quad (2.21)$$

$R_2$  is a constant. Its sign depends of the sign of the correlation  $\epsilon_c\frac{\partial^2c'}{\partial x_k^2}$  itself which could be obtained using DNS results.

- For the term of destruction due to molecular dissipation (XIII), the model proposed by Mantel & Borghi 1991 is still valid in the case of variable density. From these authors, we have:

$$2\bar{\rho}\langle d^2\frac{\partial c_{,i}}{\partial x_k}\frac{\partial c_{,i}}{\partial x_k}\rangle = \beta_0\bar{\rho}Re_t^{1/2}\frac{\langle\epsilon_c\rangle^2}{\langle c'^2\rangle} \quad (2.22)$$

$\beta_0$  is a constant ( $\beta_0 = 1.25$ ).

- concerning the production (or destruction) terms due to chemical reactions (XIV) and (XV), further investigations are in progress in order to propose new closures for these terms.

### 3. Conclusion and future plans

A transport equation for the dissipation of the fluctuation of a reactive scalar has been established in the case of variable density and variable diffusivity. The assumptions of constant pressure, no heat losses, and a Lewis number of unity significantly simplify the equation. As in the case with constant density (Mantel & Borghi 1991), an order of magnitude analysis using adequate scale relations shows



that the effects of stretching, molecular dissipation, local curvature, and chemical reactions are dominant. As a first approximation, some closure models are proposed, but further theoretical developments and comparison with DNS results must be done to confirm these models.

Analytical developments must be in the limit of large Damköhler and Reynolds numbers in order to study the relative importance of the unclosed terms.

DNS could also give essential information on the sign of some correlations and will allow the study the different terms of the equation separately. Existing DNS results of flame propagation in a decaying homogeneous turbulence for different Lewis number will be used. New computations will be performed over a large range of the ratio  $u'/S_L$  in order to assess the validity of the models and to complete the CTR DNS database.

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### REFERENCES

- ANTONIA, R. A. & BROWNE, L. W. R. 1983 The Destruction of Temperature Fluctuations in a Turbulent Plane Jet. *J. Fluid Mech.* **134**, 67-83.
- BEGUIER, C., DEKEYSER, J. & LAUNDER, B. E. 1978 Ratio of Scalar and Velocity Dissipation Time Scales in Shear Flow Turbulence. *Phys. Fluids.* **21-3**, 307-310.
- BIDAUX, E., VERVISCH, L. & BRAY, K. N. C. 1993 Study of the Transport Equation for a Surface Density Function and Some Implications for Turbulent Combustion Modelling. *Submitted for publication.*
- BORGHI, R. 1978 Réactions Chimiques en Milieu Turbulent. *Thèse de Doctorat d'Etat*, Université Pierre et Marie Curie Paris VI.
- BORGHI, R. 1990 Turbulent Premixed Combustion: Further Discussions on the Scales of Fluctuations. *Combustion and Flame.* **80**, 304-312.
- BORGHI, R. & DUTOYA, D. 1978 On the Scale of the Fluctuations in Turbulent Combustion. *Seventeenth Symp. (International) on Combust.* 235-244.
- BRAY, K. N. C. 1985 Laminar Flamelet Modelling of Turbulent Combustion. *Lecture Notes in Physics*, Springer Verlag. **241**, 3-19.
- BRAY, K. N. C. & LIBBY, P. A. 1986 Passage Times and Flamelet Crossing Frequencies in Premixed Turbulent Combustion. *Combustion, Science and Technology.* **47**, 253-274.
- BRAY, K. N. C. & MOSS, J. B. A Unified Statistical Model of the Premixed Turbulent Flame *Acta Astronautica* **4**, 291-319.
- CANDEL, S. M. & POINSOT, T. J. 1990 Flame Stretch and the Balance Equation for the Flame Area. *Combustion, Science and Technology.* **70**, 1-15.

- DUCLOS, J. M., VEYNANTE, D. & POINSOT, T. 1993 A Comparison of Flamelet Models for Premixed Turbulent Combustion. *Combustion and Flame*. **95**, 101-108.
- KERSTEIN, A. R., ASHURST, W. T. & WILLIAMS, F. A. 1988 Field Equation for Interface Propagation in an Unsteady Homogeneous Flow Field. *Physical Review*. **A-37-7**, 2728-2731.
- LIBBY, P. A. & BRAY, K. N. C. 1980 Implication of the Laminar Flamelets Model in Premixed Turbulent Combustion. *Combustion and Flame*. **39**, 33-41.
- MANTEL, T. & BORGHI, R. 1991 A New Model of Premixed Wrinkled Flame Propagation Based on a Scalar Dissipation Equation. *13th ICDERS*, Nagoya (Japan), (will appear in *Combustion and Flame*).
- MANTEL T., BORGHI R. & PICART A. 1993 Turbulent Premixed Flame Propagation Revisited Results with a New Model. *Ninth Symposium on Turbulent Shear Flows*, Kyoto (Japan).
- MARBLE, F. E. & BROADWELL, J. E. 1977 The Coherent Flame Model for Turbulent Chemical Reactions. *Technical Report TRW-9-TV*, Purdue University.
- PETERS, N. 1992 A Spectral Closure for Premixed Turbulent Combustion in the Flamelet Regime. *J. Fluid Mech.* **242**, 611-629.
- POPE, S. B. 1988 Evolution of Surfaces in Turbulence. *Int. Journal of Ing. Sciences*. **26**, 445-469.
- TENNEKES, H. & LUMLEY, J. L. 1972 A First Course in Turbulence. *The MIT Press*.
- TROUVÉ, A. & POINSOT, T. 1992 The Evolution Equation for the Flame Surface Density in Turbulent Premixed Combustion. *Proceedings of the 1992 Summer Program*. Center for Turbulence Research, Stanford Univ./NASA Ames, 325-343.
- WILLIAMS, F. A. 1985 In the Mathematics of Combustion. *SIAM Philadelphia*. 97-131.